

High-resolution spatial modelling of greenhouse gas emissions from land-use change to energy crops in the United Kingdom

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Abstract

We implemented a spatial application of a previously evaluated model of soil GHG emissions, ECOSSE, in the United Kingdom to examine the impacts to 2050 of land-use transitions from existing land use, rotational crop land, permanent grassland or woodland, to six bioenergy crops; three 'first-generation' energy crops: oilseed rape, wheat and sugar beet, and three 'second-generation' energy crops: *Miscanthus*, short rotation coppice willow (SRC) and short rotation forestry poplar (SRF). Conversion of rotational crops to *Miscanthus*, SRC and SRF and conversion of permanent grass to SRF show beneficial changes in soil GHG balance over a significant area. Conversion of permanent grass to *Miscanthus*, permanent grass to SRF and forest to SRF shows detrimental changes in soil GHG balance over a significant area. Conversion of permanent grass to wheat, oilseed rape, sugar beet and SRC and all conversions from forest show large detrimental changes in soil GHG balance over most of the United Kingdom, largely due to moving from uncultivated soil to regular cultivation. Differences in net GHG emissions between climate scenarios to 2050 were not significant. Overall, SRF offers the greatest beneficial impact on soil GHG balance. These results provide one criterion for selection of bioenergy crops and do not consider GHG emission increases/decreases resulting from displaced food production, bio-physical factors (e.g. the energy density of the crop) and socio-economic factors (e.g. expenditure on harvesting equipment). Given that the soil GHG balance is dominated by change in soil organic carbon (SOC) with the difference among *Miscanthus*, SRC and SRF largely determined by yield, a target for management of perennial energy crops is to achieve the best possible yield using the most appropriate energy crop and cultivar for the local situation.

Keywords: bioenergy, carbon, greenhouse gas, land-use change, *Miscanthus*, short rotation coppice, short rotation forestry, soil

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Introduction

Two of the greatest challenges facing humanity this century are climate change, and the need to produce enough energy to meet the demands of a growing and developing population (Edenhofer *et al.*, 2014). Bioenergy has been proposed as a potential significant contributor to both issues; as a feedstock for delivering energy security (Sims *et al.*, 2006), and as a contributor to climate mitigation, through substitution of fossil fuels, thereby reducing net greenhouse gas (GHG)

emissions from energy production (Creutzig *et al.*, 2015). Further, if the carbon dioxide (CO₂) released on combustion for energy generation was pumped into long-term geological storage (bioenergy with carbon capture and storage: BECCS), it may also serve as a negative emission technologies, capable of removing CO₂ from the atmosphere (Fuss *et al.*, 2014; Smith *et al.*, 2016). Although bioenergy is not without its limitations (Creutzig *et al.*, 2015; Smith *et al.*, 2016), its potential role in contributing to climate mitigation and energy security has led to considerable attention over recent years (Creutzig *et al.*, 2015) with some analyses suggesting that 20% of global energy demand could be met by biomass without impact on food supply (Beringer *et al.*,

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2011; Slade *et al.*, 2014). In the United Kingdom, about 3% of primary energy was from bioenergy in 2015, with bioenergy contributing 72% of all renewable energy (DECC, 2015). However, much of the current biomass feedstock for bioenergy is imported and this is expected to continue up to 2050 (Howes *et al.*, 2011). The UK Bioenergy Strategy (DECC, 2012) suggested that sustainably sourced bioenergy (i.e. not from land with high C stocks such as peatland or forest, or land used for food production) could contribute ~8–11% to the UK's total primary energy demand by 2020 and ~8–21% by 2050. If the United Kingdom is to source a proportion of this bioenergy domestically, some land-use change (LUC) to bioenergy crops is required.

It is important to assess the GHG implications of land-use transitions to bioenergy crops because LUC entails change in soil organic carbon (SOC) stocks (Smith, 2008), and also potentially, emissions of other non-CO₂ GHGs (Smith *et al.*, 2008), namely nitrous oxide (N₂O) and methane (CH₄). This will better inform decisions about what energy crops to use, what current land uses to target (and avoid) for energy crop development, and where to best to grow each crop (Alexander *et al.*, 2014; Hastings *et al.*, 2014; Wang *et al.*, 2014). To these ends, the principal objective of the spatial modelling exercise described here was to estimate the effects of land-use change (LUC) to bioenergy crops, on SOC content and GHG emissions in the United Kingdom, in order assess the impact of potential bioenergy transitions. Eighteen land-use transitions were considered:

- Rotational crops (which includes rotations consisting entirely of arable crops and also those including rotational grass) to *Miscanthus* (*Miscanthus giganteus*), short rotation coppice (SRC; here represented by willow genotype Joruun [*Salix viminalis* L. x *S. viminalis*], since this is the SRC species currently used in commercial plantations in the UK) and short rotation forestry (SRF; here represented by poplar [mixed cultivars; *Populus trichocarpa*, *deltoids*, *nigra*], since this generally shows the highest yield under UK conditions)
- Permanent grass and forest to wheat, oilseed rape (OSR), sugar beet, *Miscanthus*, SRC and SRF
- Three 'null' transitions for rotational crops, permanent grass and forest to provide results for unchanged land use as a baseline.

Conversion from rotational crops to OSR, sugar beet and wheat was not considered because the rotational crop land-use prior to transition is assumed to be similar to that following the transition, resulting in no change in net GHG balance.

Results from the spatial simulations to determine the effects of LUC transitions to bioenergy crops on SOC,

GHG emissions and net soil GHG balance in the United Kingdom are presented. Net soil GHG balance from simulations carried out using data from low, medium and high emission climate scenarios is compared to determine the impact of climate uncertainty.

Materials and methods

The ECOSSE model

The ECOSSE (Estimation of Carbon in Organic Soils – Sequestration and Emissions) model simulates soil C and nitrogen (N) dynamics in both mineral and organic soils using meteorological, land use, land management and soil data and simulates changes in SOC and soil GHG emissions. The model is able to function at the field scale or at the national scale (using only the limited data available at this scale; Smith *et al.*, 2010a,b,c).

ECOSSE was developed from concepts originally derived for mineral soils in the RothC model (Jenkinson & Rayner, 1977; Jenkinson *et al.*, 1987; Coleman & Jenkinson, 1996) and SUN-DIAL model (Bradbury *et al.*, 1993; Smith *et al.*, 1996). ECOSSE describes soil organic matter using 5 pools: inert organic matter, humus, biomass, resistant plant material (RPM) and decomposable plant material (DPM). All of the major processes of C and N turnover are included in the model, but each process is simulated using only simple equations driven by readily available inputs. This enables ECOSSE to be used for national scale simulations for which only limited input data are available.

ECOSSE simulates the soil profile to a depth of up to 3 m, dividing the soil into 5 cm layers to facilitate the accurate simulation of processes to depth. Plant C and N inputs are added monthly to the DPM and RPM pools. During the decomposition process, material is exchanged between the soil organic matter pools according to first-order equations, characterized by a specific decomposition rate for each pool. The decomposition rate of each pool is modified dependent on the temperature, water content, plant cover and pH of the soil (with additional modifiers dependent upon soil bulk density and inorganic N concentration in the case of anaerobic decomposition; Smith *et al.*, 2010c). The decomposition process results in gaseous losses of CO₂ and CH₄, with CO₂ losses dominating under aerobic conditions and CH₄ losses under anaerobic conditions. ECOSSE also simulates the oxidation of atmospheric CH₄, which, under aerobic conditions, can lead to the soil being a net consumer of CH₄ (Smith *et al.*, 2010c).

The nitrogen (N) content of the soil follows the decomposition of the soil organic matter, with a stable C:N ratio defined for each soil organic matter pool at a given pH, and N being either mineralized or immobilized to maintain that ratio. Nitrogen is released from decomposing soil organic matter as ammonium (NH₄⁺) and may be then immobilized or nitrified to nitrate (NO₃⁻). Carbon and N may be lost from the soil by the processes of leaching of NO₃⁻, dissolved organic C, dissolved organic N, denitrification to nitric oxide (NO) and N₂O, volatilization of ammonia, or crop off-take of NO₃⁻ and NH₄⁺. Carbon and N may be returned to the soil by plant input, application of inorganic fertilizers, atmospheric deposition or organic amendments (e.g. manure, crop residues).

ECOSSE simulates the soil water content of each layer using a 'tipping bucket' approach based on the SUNDIAL model (Bradbury *et al.*, 1993; Smith *et al.*, 1996). Water from precipitation entering the soil forces water in the soil deeper into the soil profile. Precipitation fills the uppermost soil layer with water until it reaches field capacity. Any remaining precipitation is then used to fill the next layer to field capacity. This process is repeated until no precipitation remains or the bottom of the profile is reached. Any precipitation water remaining after filling all layers to field capacity is partitioned between drainage (water leaving the soil profile) and excess, which is used to fill layers to saturation from the bottom of the profile upwards. This is performed using the observed depth of the water table, the available water at saturation and weather data to calculate the restriction to drainage (i.e. the fraction of the remaining water that becomes excess), that is required to achieve the observed water table depth. Water is also lost from the top of the profile as evapotranspiration, which is estimated using the Thornthwaite (1948) method.

The ECOSSE model has been thoroughly evaluated and shown to simulate SOC change, N₂O and CH₄ emissions reliably, for bioenergy crop transitions in the United Kingdom using field data from *Miscanthus*, SRC and SRF field sites, as described in Dondini *et al.*, 2015, 2016a,b).

Spatial application of the ECOSSE model

The spatial simulations of the United Kingdom are carried out on a 1 km grid basis giving a total of nearly 0.25 million grid cells. Grid cells which contain inappropriate land for growing bioenergy crops were excluded from the simulations based on the UKERC 7 land-use constraints (Lovett *et al.*, 2014). The UKERC 7 constraints mask excludes 100 m grid cells that meet one or more of the following criteria (Lovett *et al.*, 2014): slope $\geq 15\%$; peat (soil C $\geq 30\%$); designated areas; urban areas, roads, rivers; parks; scheduled monuments/world heritage sites; woodland and natural habitats from LCM2007 (including acid, neutral and calcareous grassland). We aggregated the UKERC 7 mask to 1 km, using the mode of the 100 m cells to determine exclusions at the 1 km scale. We also disaggregated the woodland category in order to permit use of woodland for transitions to SRF; we term this mask UKERC 7w. The land-use data that were used to initialize the ECOSSE 1 km grid were aggregated using the mode from the LCM2007 land cover from at 1 ha resolution in the UKERC mask (Lovett *et al.*, 2014).

The simulation of each LUC was carried out for up to 5 different soil types in each grid cell to capture soil heterogeneity at the subgrid cell level. All combinations of LUC from rotational crops, permanent grass and forest to wheat, OSR, sugar beet, *Miscanthus*, SRC and SRF were simulated, except for rotational crops to wheat, OSR and sugar beet which, being types of rotational crops, were considered to be equivalent to no LUC. Three 'null' transitions for rotational crops, permanent grass and forest were also simulated to provide results for unchanged land-use for comparison.

The rotational crop land-use category represents land used to grow arable crops and includes all-arable rotations and rotations that include rotational or temporary grassland for part of

the rotation. The permanent grass land-use category represents permanent, uncultivated grassland only. Rotational grass is not a land-use and is part of rotational farming better represented by the rotational crops category (which may include periods of rotational grass).

Results were obtained using three different climate scenarios for a 35-year period running from 2015 to 2050. Prior to each simulation, the model was initialized to partition the SOC into the different SOC pools based on the assumption that the SOC in the soil column is at steady state under the land use given for the start of the simulation.

Following initialization, the main simulation was executed. This started with LUC from the initial land-use type to the bioenergy crop. Any soil cultivation carried out during LUC was simulated. As rotational cropland typically undergoes annual cultivation, the model assumes there is no additional cultivation required for the establishment of bioenergy crops. In contrast, the model simulates soil cultivation for LUC from permanent grass and forestry because these land-use types typically require ground preparation before bioenergy crops are planted. The model simulates physical fragmentation of soil organic matter resulting from cultivation by moving a proportion of the C and N in the humus pool, (which has a slow decomposition rate), to the DPM and RPM pools (which have faster decomposition rates; Smith *et al.*, 2010a). Redistribution of soil organic matter during cultivation is simulated by homogenizing the vertical distribution of the soil organic matter pools down to the cultivation depth – which might be expected with inversion ploughing followed by harrowing as ground preparation. The simulated cultivation depth for conversion from forest and permanent grass is 0.5 and 0.3 m, respectively.

After simulation of the cultivation associated with LUC, the model simulates soil dynamics under the bioenergy crop. The annual plant inputs of C and N to the soil are calculated from the annual yield of the crop (provided as an input to the model), using crop-specific ratios estimated from the literature.

For perennial bioenergy crops, the model simulates annual yield dynamics over the lifetime of the crop to account for reduced yields during establishment and peak yield later in the crop life cycle. Yield dynamics are modelled using the lifetime mean annual yield of the crop (as an input to the model) and five crop-specific parameters:

- $Y_{\text{peak-ratio}}$ – ratio of peak annual yield to lifetime mean annual yield, used to calculate peak annual yield.
- T_{peak} – time required for the crop to reach peak annual yield.
- T_0 – time spent at initial yield, before annual yield begins to increase towards peak annual yield. Used to approximate a sigmoidal growth curve.
- $Y_{0-\text{frac}}$ – initial yield as a fraction of lifetime mean annual yield. This parameter is calculated from the other parameters to ensure that the lifetime mean annual yield of the crop is preserved.
- Lifetime – the lifespan of the crop.

The parameter values for each perennial crop, which are based on expert opinion and informed by published studies

Table 1 Yield model parameters for *Miscanthus*, SRC and SRF. See text for an explanation of each parameter

Crop	$Y_{\text{peak-ratio}}$	T_{peak} (years)	T_0 (years)	$Y_{0-\text{frac}}$	Lifetime (years)
<i>Miscanthus</i>	1.1	5	0	0.299	20
SRC	1.1	6	0	0.433	20
SRF	1.6	15	4	0.267	20

such as Arundale *et al.* (2014), are given in Table 1. The simulated yield dynamics are characterized by 3 stages: a period spent at initial annual yield (SRF only), a period of linearly increasing annual yield and a period spent at peak annual yield. An example of the growth dynamics of each crop given by the parameter values in Table 1 is shown in Fig. 1. The lifetime mean annual yields used as an input to the model are taken from a number of sources described below.

The annual yield dynamics of perennial crops typically follow a sigmoidal curve. Here, we employed a simple linear-based approach to yield modelling to maintain model parsimony. *Miscanthus* and SRC establish quickly and do not have a very pronounced sigmoidal growth curve. Therefore, the linear increase during establishment will only result in a small error in the timing of plant inputs to the soil (and subsequent effects on the timing of changes in SOC and GHG emission). For SRF, which has a longer establishment time and a more pronounced sigmoidal growth curve, we introduced an additional flat growth phase at the start of establishment to better approximate the sigmoidal curve and minimize the error in the timing of plant inputs.

Each perennial bioenergy crop was re-established after a 20-year period (the estimated productive lifespan of the crop). It is assumed that re-establishment does not involve further cultivation. This assumption was made because perennial bioenergy crops can be re-established with only shallow soil disturbance

or very localized soil disturbance (McCalmont *et al.*, 2015). *Miscanthus* crops can be re-established by herbicide application of the existing crop followed by direct drilling of rhizomes, or planting plugs grown from seed (Clifton-Brown *et al.*, 2015). Ploughing of *Miscanthus* can be avoided by exposing the rhizomes on top of the soil so that they dehydrate and die (Caslin *et al.*, 2011a). The SRC can be removed by application of herbicide followed by mulching of the stools (using a bush-hogger), into the top 5–10 cm of the soil (Defra, 2004) and SRF may be re-established by planting between previous stumps (McKay, 2011). The impacts of soil disturbance during re-establishment of perennial bioenergy crops are poorly understood and require further research (Grogan & Matthews, 2002). However, as the re-establishment of these crops can be made with only shallow soil disturbance (the top 5–10 cm), or very localized disturbance (e.g. direct drilling of *Miscanthus* and replanting SRF between stumps), we expect the impacts on SOC to be small. Fertilizer was applied to *Miscanthus* and SRC at an annual rate of 30 and 60 kg N ha⁻¹, respectively, following recommended practice (Defra, 2010; Caslin *et al.*, 2011a). Fertilizer was applied to SRF at a rate of 45 kg N ha⁻¹. No fertilizer was applied to *Miscanthus*, SRC and SRF during the first 2 years after planting, again following best practice guidelines (Defra, 2010; Caslin *et al.*, 2011a).

Forest was assumed to be unfertilized. Rotational crops, permanent grass, wheat, OSR and sugar beet were assumed to be fertilized at a rate equal to the annual crop N demand. Crop N demand is a function of plant yield and the C:N ratio of the plant. Modelled crop N demand is high for wheat because it has a low C:N ratio and a relatively high yield. In contrast, modelled N demand for permanent grass was significantly lower because it has a higher C:N ratio.

For all land-use types, the changes in SOC and emissions of GHGs were calculated for the top metre of the soil profile. Only the top metre was considered because this is the depth to which soil parameters are provided by the Harmonised World Soil Database (HWSD; see below). Changes in SOC, CH₄ and

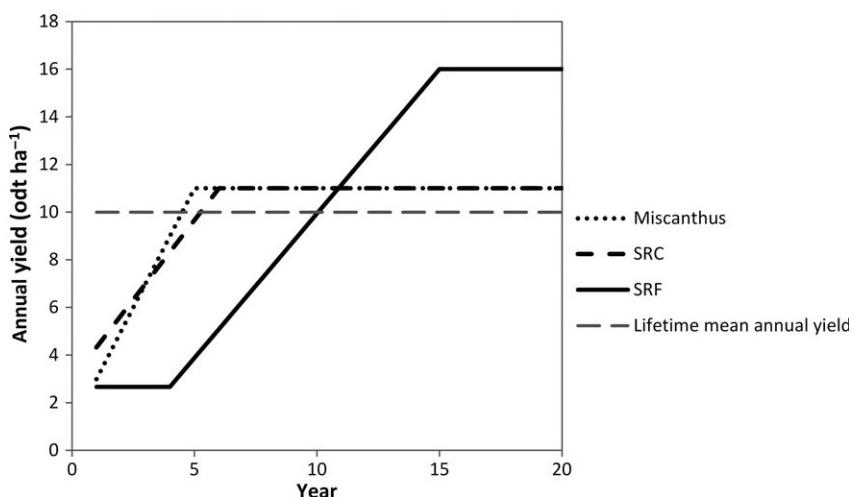


Fig. 1 Annual yield dynamics of *Miscanthus*, SRC and SRF over the 20-year lifespan of each crop, with a lifetime mean annual yield of 10 odt ha⁻¹. Lifetime mean annual yield is represented by the dashed grey line for comparison.

N_2O resulting from LUC were calculated by subtracting the results of the appropriate null transition from the LUC results, so that the change could be attributed solely to the LUC. For example, to calculate the impact of LUC from permanent grass to SRC, the results from the permanent grass null transition (i.e. grass remaining as grass) were subtracted from the permanent grass to SRC results. Each grid cell value in the model output represents the area-weighted mean of the simulations carried out for each soil type in the grid cell.

Results are given for the whole of the United Kingdom on a 1 km grid basis and express the area-weighted average obtained from simulations of the 5 most dominant soil types in each grid cell. For consistency and ease of comparison, all results (i.e. CH_4 , N_2O , change in SOC and net GHG balance) are reported in terms of CO_2 -equivalent values (CO_2e), using IPCC 100-year global warming potentials (GWP; IPCC, 2001). More recent IPCC reports have provided updated GWP from those given in the IPCC 2001 report, although, for consistency with national inventory GHG emission estimates, we have used the IPCC 2001 GWP values, following the recommended practice for national GHG inventories. Results show the cumulative total of each output variable and are relative to the value obtained if no transition had occurred (hence results directly show the effect of the transition).

Soil data

The HWSD version 1.2 was used to provide initial soil conditions in the model (FAO/IIASA/ISRIC/ISS-CAS/JRC, 2012). The HWSD provides soil data to a depth of 1 metre at a resolution of 30 arc s (approximately 1 km), for the dominant soil types in each grid cell; we reprojected this to the British National Grid using methods described by Ordnance Survey (Ordnance Survey, 2010). The soil properties used from this database to drive ECOSSE were as follows: organic C content, bulk density, pH, and sand, silt and clay fraction. The HWSD does not include information on the water-holding capacities of soils so these were estimated using British Soil Survey pedotransfer functions (Hutson & Cass, 1987), which performed well in evaluations (Donatelli *et al.*, 1996; Givi *et al.*, 2004). The HWSD also provides the percentage of grid cell area covered by each soil type. The ECOSSE model is run for each dominant soil type in each grid cell and the output area-weighted by the percentage cover in each grid cell to calculate its mean response.

Climate data

ECOSSE requires precipitation and air temperature data which are used to drive the soil water model and to determine temperature-based rate modifiers for various soil processes. The meteorological driving data was taken from the UKCP09 Spatially Coherent Projections (Murphy *et al.*, 2009). UKCP09 provides average monthly temperature and precipitation in a 25 km grid for overlapping 30-year periods centred on decades ranging from the 2020s to the 2080s, for high, medium and low emissions scenarios; again, we reprojected this to the British National Grid using methods described by Ordnance Survey (Ordnance Survey, 2010).

Yield data

ECOSSE requires yield data for each land-use type in order to estimate the monthly plant inputs to the soil. Yield data for the bioenergy crops have been obtained from a range of sources of varying spatial resolution. Baseline yields for first-generation crops were obtained from EUROSTAT (2014), which provides mean wheat and OSR yields across 12 NUTS (Nomenclature of Territorial Units for Statistics) regions in the United Kingdom, and a single mean national yield for sugar beet, based on Defra farm surveys. The baseline yield values for the rotational crop land-use category follow those of wheat.

Yield estimates for wheat, OSR and sugar beet under different climate scenarios were obtained by adjusting the baseline yields using the Miami model (Lieth, 1975). Miami is an empirical net primary production (NPP) model that estimates annual NPP from mean annual temperature and annual precipitation. The Miami estimate of NPP was calculated for each decade in each grid cell using the same UKCP09 climate data that was used for the ECOSSE simulations. The percentage change in NPP relative to the baseline Miami NPP was applied to the baseline yield data to adjust the yield for each climate scenario. Yield estimates for permanent grass and forest are obtained using NPP estimates from Miami, which are then linearly rescaled according to observed peak yields (Living Countryside, 2013) to reflect differences in grass and forest productivity.

Lifetime mean annual yield estimates for *Miscanthus*, SRC and SRF were obtained from simulations using the models MiscanFor (Hastings *et al.*, 2009), ForestGrowth SRC (Tallis *et al.*, 2013) and ESC-CARBINE (Thompson & Matthews, 1989; Pyatt *et al.*, 2001), respectively. The yield predictions have been obtained using the same UKCP09 climate and HWSD soil data used as inputs to ECOSSE. These models were used due to their validated accuracy and use of compatible data. The lifetime mean annual yields were provided for each decade because the UKCP09 climate data provide long-term average climate values centred on each decade. As an ECOSSE simulation progresses, the annual yield for each year of the simulation is calculated from the lifetime mean annual yield for the current decade. Therefore, if the lifetime mean annual yield changes between decades, this is reflected by a change in the annual yield calculated within the model.

SRC was represented by willow. Although the yield modelling study of Hastings *et al.* (2014) found that SRC poplar outperformed SRC willow in almost all regions within Great Britain, willow remains the SRC species currently used in commercial plantations in the United Kingdom and thus, despite lower yields, is used to represent SRC here. SRF was represented by poplar, because Hastings *et al.* (2014) found that poplar outperformed all other SRF species included in the study except for Sitka spruce in the Scottish Highlands and Pennines (areas which are mostly excluded by the UKERC constraints mask). The other SRF species included in the study were as follows: aspen (*Populus tremula* L.), black alder (*Alnus glutinosa* L.), European ash (*Fraxinus excelsior* L.), sitka spruce (*Picea sitchensis* [Nong.] Carr.) and silver birch (*Betula pendula* Roth). The lifetime mean annual yields of SRF poplar across Great Britain were at least double those of other species. Given

no clear commercial benefits of selecting other SRF species over poplar, we assumed the strong commercial incentive offered by the much higher yields will mean that poplar will be the dominant SRF species in the United Kingdom. Planting of lower yielding SRF species to avoid pest and disease outbreaks would result in consequent lower inputs to the soil.

The spatial distributions of yield used for each crop as driver for the ECOSSE model runs are presented in Fig. 2, showing mean annual yields in a single decade (2030s). Mean decadal yields changed by <2 oven dry tonnes (odt) $\text{ha}^{-1} \text{yr}^{-1}$ over the 35-year study period for any single crop (data not shown).

If LUC leads to an increase in plant C inputs to the soil, the SOC content will gradually increase over time until a new equilibrium SOC content is reached (assuming all other factors remain equal). In ECOSSE, the quantity of new plant material entering the soil organic matter pools is determined by the amount of plant biomass (calculated from yield), minus the proportion of biomass that is removed during harvest.

Across the simulation area, SRF, *Miscanthus* and sugar beet are the highest yielding bioenergy crops with United Kingdom mean annual yields of 10–12 odt ha^{-1} . Based on reported harvest index values (Table 2), the model assumes that 75% of sugar beet biomass is removed during harvest, compared with

64% for *Miscanthus* and 60% for SRF. The low harvest index (relative to sugar beet) and high yields mean that SRF and *Miscanthus* have, on average, higher plant inputs to the soil than other bioenergy crops.

Conversion to bioenergy crops can also lead to a change in the quality of plant inputs to the soil. Plant residues from perennial grasses and woody plants such as *Miscanthus*, SRC and SRF are typically slower to decompose than residues from annual crops such as wheat, OSR and sugar beet (due in part to the residues having a higher C:N ratio). Slower decomposition rates reduce the rate of SOC loss. In the model, differences in crop residue decomposition rates are simulated through differential allocation of plant residues to two SOC pools: the DPM and RPM pools. The DPM pool has a faster decomposition rate than the RPM pool. To reflect the slower decomposition rates, residues from *Miscanthus*, SRC and SRF have a higher RPM:DPM ratio than residues from wheat, OSR and sugar beet.

Results

Differences in net GHG balance between the climate scenarios for land-use transitions to bioenergy crops are

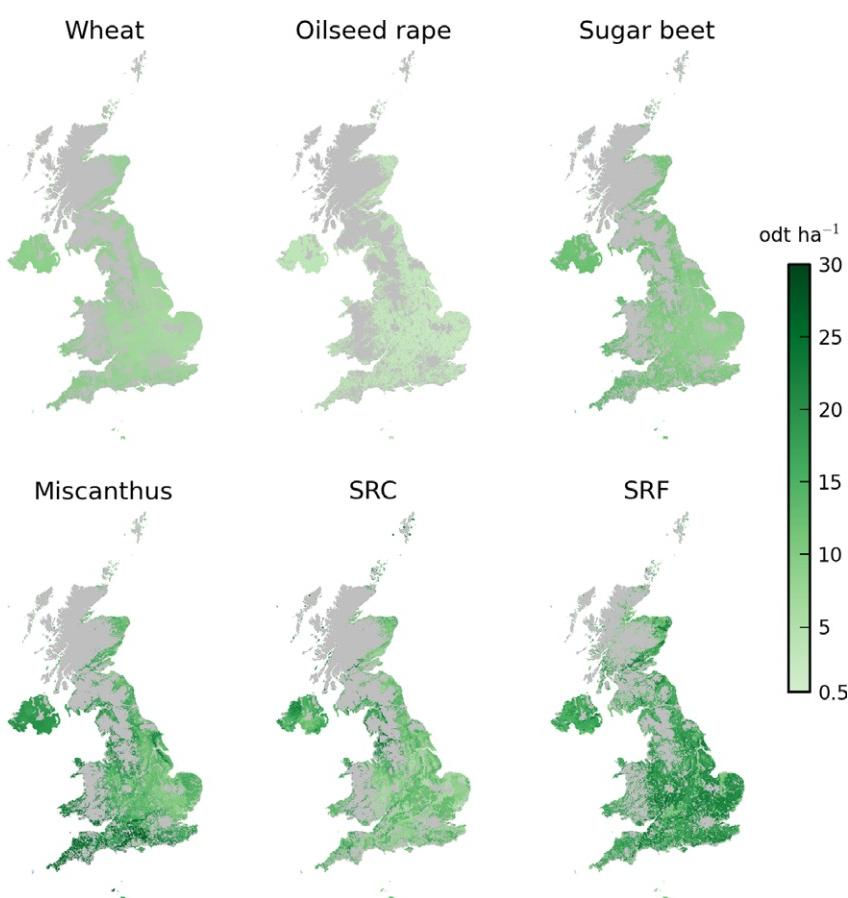


Fig. 2 Spatial distribution of modelled mean annual yield of bioenergy crops as $\text{odt ha}^{-1} \text{yr}^{-1}$ (where odt is oven dry tonnes) in the 2030s under the UKCP09 medium emissions climate scenario. *Miscanthus*, SRC and SRF yields were obtained from simulations using the models MiscanFor, ForestGrowth SRC and ESC-CARBINE, respectively. Defra yield statistics from 2000 to 2008 were used to establish baseline yield values for wheat, OSR and sugar beet, which were then adjusted for future climate using the Miami model (see text).

Table 2 Harvest index parameter values of bioenergy crops. Note that the wheat harvest index includes the harvest of both grain and straw

Crop	Harvest index	Source
<i>Miscanthus</i>	0.64	Zhuang <i>et al.</i> (2013)
Oilseed rape	0.35	Kjellström & Kirchmann (1994), Drecer <i>et al.</i> (2000), HGCA (2014)
SRC	0.6	Caslin <i>et al.</i> (2011b)
SRF	0.6	No data available so assumed to be the same as SRC
Sugar beet	0.75	Tsialtas & Karadimos (2003), Ortiz <i>et al.</i> (2012)
Wheat	0.77	White & Wilson (2006), Stoddart & Watts (2012)

very small in comparison with the effects of LUC, being within $\pm 2 \text{ t CO}_2\text{e ha}^{-1}$ over the 35-year period for any given transition. Given this very minor impact of climate to 2050, all results presented are for the medium climate scenario, and all results refer to the period 2015–2050 unless otherwise stated.

Net GHG balance represents the combined effects of changes in N_2O , CH_4 and SOC and is therefore the most comprehensive measure of bioenergy impacts; a negative GHG balance represents removals from the atmosphere (i.e. beneficial), and a positive GHG balance represents emissions to the atmosphere (i.e. detrimental). Only second-generation bioenergy crops (*Miscanthus*, SRC and SRF) showed any beneficial changes in soil GHG balance; all conversions to first-generation bioenergy crops (wheat, sugar beet and OSR) showed a detrimental impact on net GHG balance (Figs 3–5), except of course for ‘conversion’ from rotational crops, where a null transition is assumed (i.e. zero GHG balance).

Of the three initial land uses, conversion from rotational crops has the most favourable net GHG balance (Fig. 3). Conversion of rotational crops to SRF, SRC and *Miscanthus* each showed a beneficial response in almost all grid cells, with mean net GHG balance values of -126.9 , -37.8 and $-76.4 \text{ t CO}_2\text{e ha}^{-1}$ over 35 years, respectively. In contrast, all conversions from permanent grass result in a detrimental change in net GHG balance in all grid cells except for SRF, which shows a small beneficial ($>-21 \text{ t CO}_2\text{e ha}^{-1}$) change over large parts of the West Midlands, East Midlands and East Anglia (Fig. 4). Transitions from forest show detrimental soil net GHG balance in all grid cells with mean values of 88.7 , 128.6 and $102.9 \text{ CO}_2\text{e ha}^{-1}$ over 35 years for SRF, SRC and *Miscanthus*, respectively (Fig. 5). Overall, conversion of rotational crops to SRF is the most favourable conversion because it has the most beneficial net GHG balance over the largest area (Fig. 3). However, in some areas, most notably in parts of south-west England, southern England, south and west Wales, and in a narrow band north and south of the Humber, *Miscanthus* presents an equal or slightly better bioenergy opportunity than SRF (see the Discussion for further consideration of this). In contrast, SRC does not show a more beneficial net GHG balance than SRF or *Miscanthus* in any areas of significant size (Fig. 3).

The mean, minimum and maximum cumulative changes in SOC (expressed as loss of SOC, i.e. CO_2 emissions), in N_2O emissions and in CH_4 emissions from 2015 to 2050 following LUC from rotational crops, permanent grass and forest to all energy crops are shown in Table 3.

Conversion of land to bioenergy crops shows a large spatial and temporal variation in net GHG balance and its components: SOC, N_2O and CH_4 . The impact of land-use change on net GHG balance depends upon the

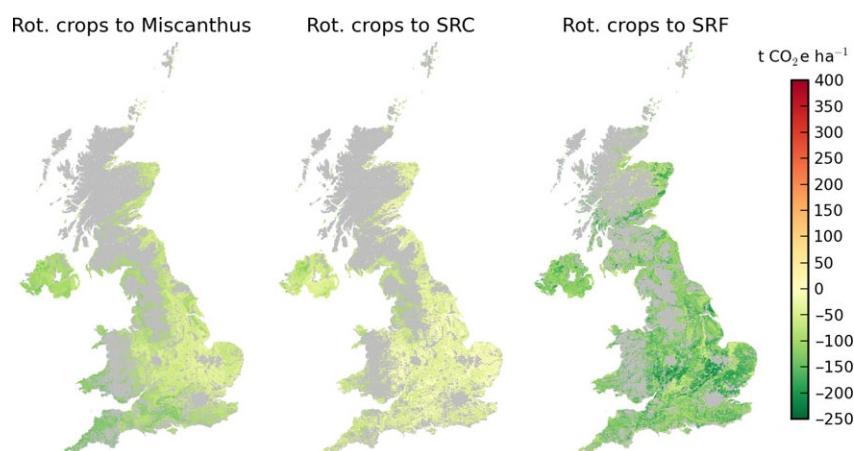


Fig. 3 Greenhouse gas emissions when rotational crops are converted to second-generation energy crops.

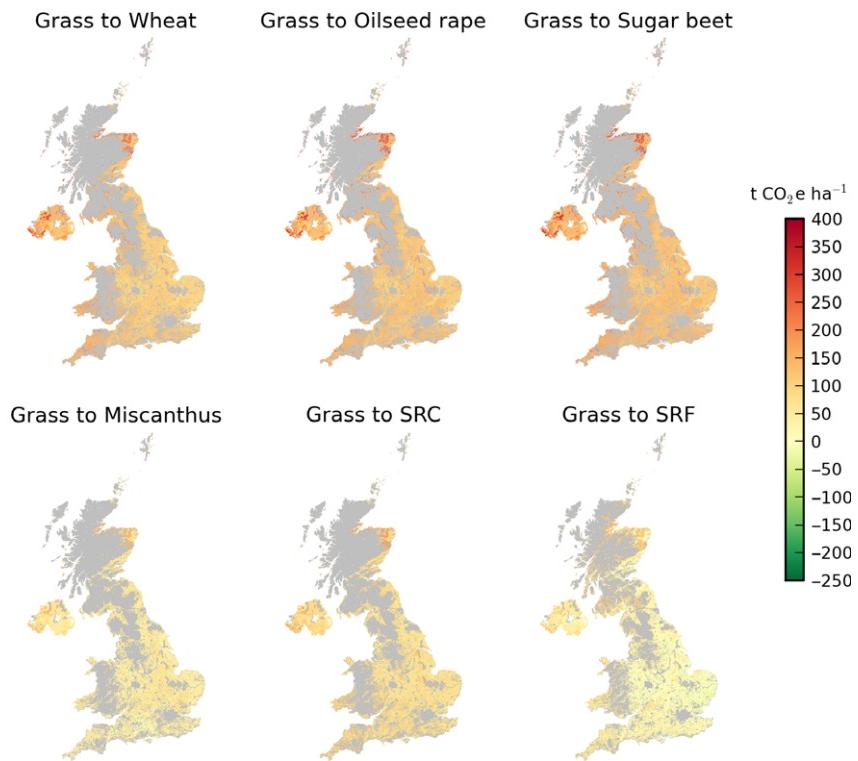


Fig. 4 Greenhouse gas emissions when permanent grass is converted to energy crops.

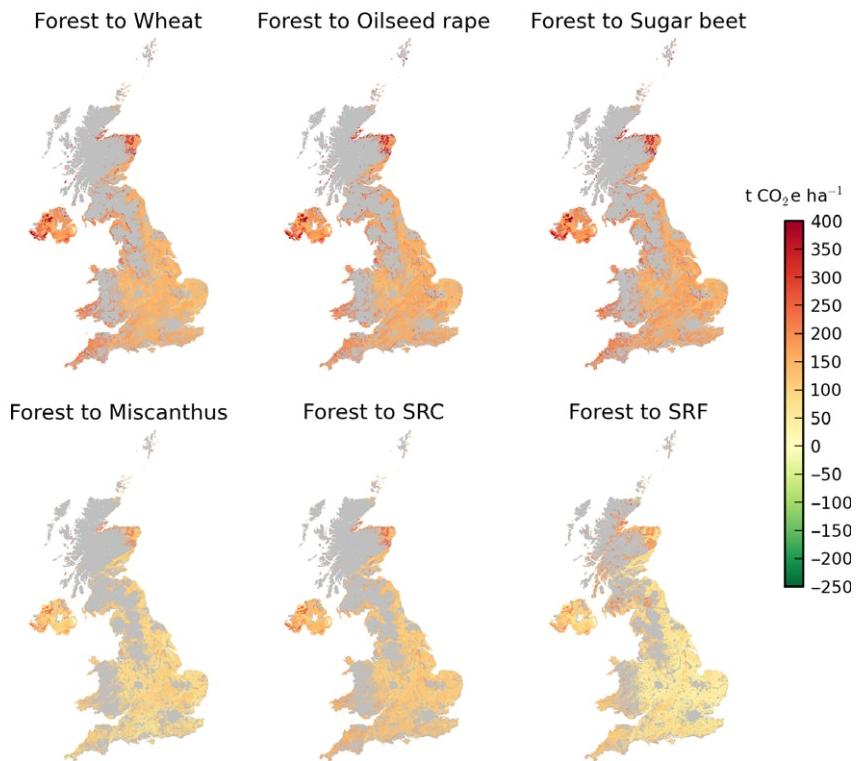


Fig. 5 Greenhouse gas emissions when forest is converted to energy crops.

Table 3 Mean (minimum and maximum range in parentheses; all t CO₂e ha⁻¹) change in SOC, N₂O emissions and CH₄ emissions from 2015 to 2050, following conversion to energy crops from rotational crops, permanent crops, grassland and forest. All positive values are emissions to the atmosphere, so an SOC gain (removal of CO₂ from the atmosphere) is shown as negative

		Energy crop (all cumulative emissions in t CO ₂ e ha ⁻¹ for 2015–2050)					
Flux	Previous land use	Wheat	OSR	Sugar beet	Miscanthus	SRC	SRF
SOC	Rotational crops	n/a	n/a	n/a	-55.4 (-121.8 to 0.7)	-18.7 (-114.4 to 27.4)	-102.9 (-205.4 to -9.9)
SOC	Grassland	85.4 (37.8 to 220.6)	119.9 (65.3 to 283.5)	118.6 (64.2 to -282.5)	44.7 (-1.7 to 147.8)	70.0 (33.0 to 186.3)	24.3 (-30.2 to 147.1)
SOC	Forest	117.9 (56.8 to 321.5)	149.7 (81.6 to 369.0)	148.5 (80.6 to 365.4)	78.2 (31.0 to 216.8)	102.0 (56.6 to 251.8)	64.0 (4.6 to 219.1)
N ₂ O	Rotational crops	n/a	n/a	n/a	-21.0 (-33.6 to -13.2)	-19.0 (-30.8 to -12.5)	-24.0 (-37.3 to -15.8)
N ₂ O	Grassland	35.9 (23.6 to 74.8)	10.9 (-0.6 to 54.3)	20.5 (10.3 to 62.1)	8.8 (0.2 to 43.9)	10.5 (1.6 to 49.2)	8.6 (-2.1 to 44.2)
N ₂ O	Forest	52.4 (39.0 to 88.0)	27.3 (16.8 to 56.4)	36.9 (25.4 to 66.5)	24.7 (13.6 to 42.9)	26.6 (17.9 to 47.7)	24.7 (16.5 to 42.3)
CH ₄	Rotational crops	n/a	n/a	n/a	0.02 (-1.10 to 0.10)	-0.03 (-1.03 to 0.03)	-0.04 (-1.22 to 0.02)
CH ₄	Grassland	-0.04 (-0.12 to 1.02)	-0.11 (-0.19 to 0.56)	-0.11 (-0.19 to 0.68)	-0.02 (-0.11 to 0.43)	-0.07 (-0.14 to 0.09)	-0.05 (-0.14 to 0.37)
CH ₄	Forest	-0.02 (-0.10 to 1.78)	-0.09 (-0.18 to 0.74)	-0.09 (-0.18 to 0.89)	0.00 (-0.06 to 0.48)	-0.05 (-0.13 to 0.81)	-0.02 (-0.13 to 0.50)

type of land-use being converted, the type of bioenergy crop planted, the geographic location and the time since conversion. Overall, changes in SOC content have the largest impact on net GHG balance, followed by changes in N₂O, then CH₄ emissions (Table 3).

Figure 6 shows the SOC, N₂O and CH₄, respectively, for one transition, rotational crops to SRF, to show the relative influence of each component on the total net GHG balance (Fig. 6).

In general, most of the benefits to net GHG balance from favourable conversions are realized in the first 15–20 years following conversion; after this time, the rate of decrease in net GHG balance declines as SOC content approaches a new equilibrium (Fig. 7).

The changes in mean cumulative net GHG balance in soil emissions over time for each land-use transition are shown in Fig. 7. Conversion from rotational crops to *Miscanthus*, SRC and SRF show a decrease in net GHG balance in soil emissions over the 35-year simulation period, although there is little change during the first 5 years following conversion of rotational crops to SRC (Fig. 7). By contrast, all conversions from permanent grass and forest show a rapid increase in net GHG balance in soil emissions 5 years after LUC (Fig. 7). After the first 5 years, the net GHG balance of most LUCs continues to increase at a slower, broadly linear rate. However, in 2030 (15 years after conversion), the net GHG balance of permanent grass to SRF begins to decrease (Fig. 7).

Discussion

Land-use change emissions, such as those reported here, make a significant contribution to the overall GHG balance of energy crop transitions and are a relatively poorly constrained term in many bioenergy life cycle analyses. We discuss our findings further below.

Effects of land-use change

Conversion of land to bioenergy crops shows a large spatial and temporal variation in net GHG balance and its components; SOC, N₂O and CH₄. The impact of LUC on net GHG balance depends upon the type of land-use being converted, the type of bioenergy crop planted and the geographic location. Overall, changes in SOC have the largest impact on net GHG balance in soil emissions, followed by N₂O and then CH₄, accounting for the GWP of each flux.

Changes in soil organic carbon

Results for 2015 to 2050 show that both the initial and target land-use type have a very large impact on mean

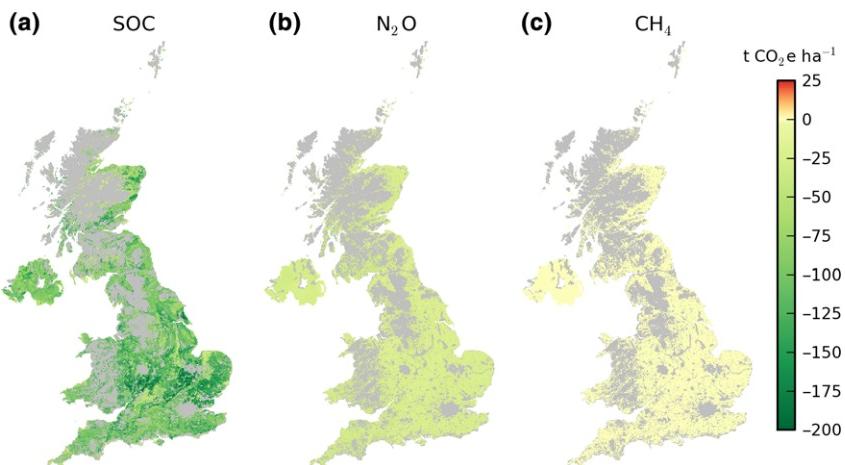


Fig. 6 All panels show the transition from rotational crops to SRF: panels a, b and c show maps of CO₂e for SOC (a), N₂O (b) and CH₄ (c).

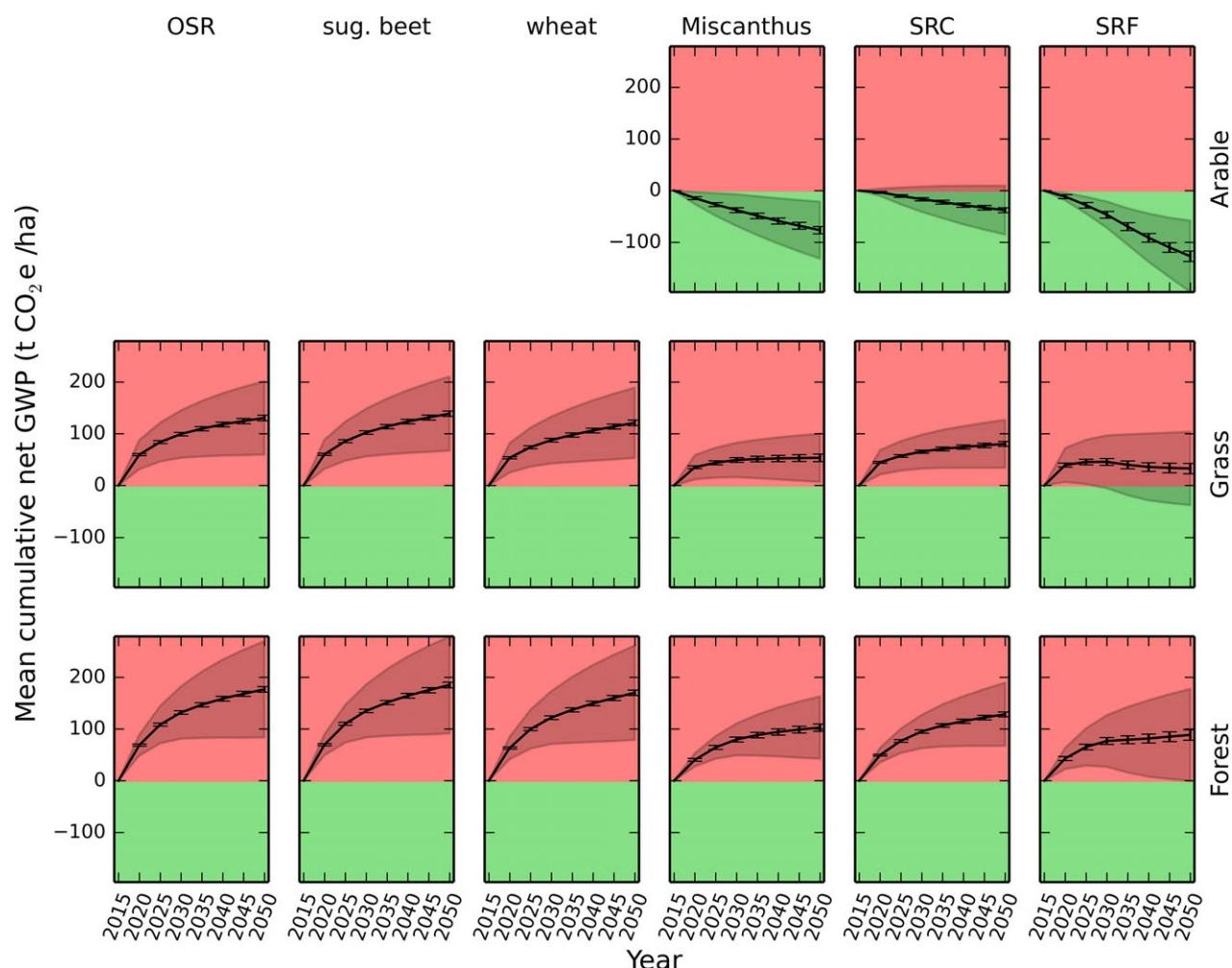


Fig. 7 Time series of mean cumulative net GHG balance resulting from land-use change to bioenergy crops in 2015 under the medium emissions climate scenario. Shaded areas show the 95% confidence interval of the distribution of modelled results (due to spatial variation) from the simulations across the United Kingdom. Error bars show the 95% confidence interval of estimated error based on the comparison of modelled and measured net GHG balance from site-level modelling studies (Dondini *et al.*, 2015, 2016a,b). The red portion of each panel shows a net GHG emission, the green portion shows a net GHG sink.

change in SOC. Conversion of rotational crops to *Miscanthus*, SRC and SRF and conversion of permanent grass to SRF are the only LUCs that lead to extensive beneficial changes in SOC. By contrast, all conversions from permanent grass to non-SRF bioenergy crops and all conversions from forest lead to mostly detrimental changes in SOC. These findings are broadly in-line with those of empirical and other modelling studies. Guo & Gifford's (2002) review of data from 74 LUC publications shows that conversion from arable land to plantation forest, secondary forest and pasture leads to significant increases in SOC, whereas conversion of forest and pasture to crop leads to large decreases. Murty *et al.* (2002) and Wei *et al.* (2014) also reported significant decreases in SOC following conversion of forest to cultivated agricultural land. For bioenergy crop transitions, the recent meta-analysis of Harris *et al.* (2015) that reported only empirical and not modelled data revealed in contrast to the findings here, broadly neutral SOC following LUC from grassland to SRC. For LUC from grassland to *Miscanthus*, the meta-analysis supports the findings here with SOC declining by 10.9 (± 4.3) %. The literature survey of McCalmont *et al.* (2015), of the environmental impact of *Miscanthus* plantations, showed a significant increase in SOC when LUC from arable and a slight decrease for LUC from grasslands. The time-scale of SOC losses in these studies was similar to those in our study, with most of the SOC loss occurring in the first 10–20 years after conversion. After this period, rates of SOC loss decline as the SOC approaches a new equilibrium.

Cultivation. As rotational cropland typically undergoes frequent cultivation, the model assumes that no additional cultivation is required for the establishment of bioenergy crops. By contrast, the model simulates soil cultivation for conversion of permanent grass and forestry because these land uses typically require ground preparation before bioenergy crops are planted. Cultivation of relatively undisturbed soil, such as soil under permanent grass and forest, usually has a large detrimental impact on SOC (Guo & Gifford, 2002), and McCalmont *et al.* (2016) also showed a slight decrease in SOC for LUC from grasslands. Cultivation physically fragments and redistributes soil organic matter, accelerating its decomposition, leading to a large release of CO₂ and subsequent decrease in SOC (Grandy & Robertson, 2006). As a rule, minimizing soil disturbance to the extent possible will minimize adverse impacts on SOC. The model captures this loss of SOC by simulating cultivation as described in the Methods section. This cultivation is responsible for the large detrimental change in SOC following LUC from permanent grass and forest (Figs 4 and 5). However, in the case of

perennial *Miscanthus*, SRC and SRF, this cultivation occurs only once for each 20-year crop cycle. It is possible in some cases for this detrimental effect to diminish slightly over time, where a higher yielding crop may produce greater SOC inputs than the previous land use, thus counterbalancing to some extent the effect of the initial soil disturbance, as evident in the grass to SRF transition in Fig. 7.

Plant inputs. The difference in quantity and quality of plant inputs is the principal reason behind the different SOC responses shown by each bioenergy crop type. As the quantity of plant inputs is partially based on yield, the spatial pattern of change in SOC broadly reflects the spatial pattern of yield. This is particularly apparent with *Miscanthus*, which shows a distinct area of high yield (as estimated by the MisanFor model) in southern England and north and south of the Humber estuary (Figs 3–5), with a corresponding large increase in SOC in these areas following conversion from rotational crops (Fig. 3). The high yields in these two areas are due to the prevalence of chalky soils with high soil water-holding capacities, which the MisanFor model predicts are favourable for the growth of *Miscanthus* (only MisanFor treats these chalky soils differently). As SOC change is largely determined by yield (with higher yields giving higher C returns to the soil than lower yields), low yields can lead to a decline in SOC. The relatively detrimental impact of the permanent grass to SRC transition is largely driven by low predicted yields of SRC willow (see Fig. 2). A target for management of perennial energy crops is, therefore, to achieve the best possible yield by selecting the most appropriate energy crop and cultivar for the local situation, as long as this can be made without excessive N fertilizer use, which would lead to increased N₂O emissions. The difference between potential and reported yields in these second-generation bioenergy crops – the so-called *yield gap* remains large (Allwright and Taylor, 2015), reflecting the limited artificial selection and breeding in these crops, compared to annual food crops and suggesting that future yield increase may be dominated by the supply of new germplasm through next-generation molecular breeding using techniques such as genome editing (Allwright and Taylor, 2015). Improved yield would have a large impact on the results reported here.

Changes in N₂O emissions

Beneficial changes in N₂O emissions following conversion of rotational crops to *Miscanthus*, SRC and SRF occur because of reductions in N fertilizer inputs. In ECOSSE, reduced N fertilizer inputs lead to decreased N₂O emissions because: (a) the denitrification rate slows

as the NO_3^- concentration in the soil decreases and (b) the proportion of denitrified N emitted as N_2O decreases as NO_3^- concentration in the soil decreases. In contrast to conversions from rotational crops, conversion of forest to wheat shows the greatest increase in N_2O because it involves a transition from a land-use that receives no fertilizer to a crop that receives a large amount of fertilizer (due to wheat's high N demand).

Beneficial changes in N_2O emissions following conversion from rotational crops show larger reductions in N_2O emissions in the west of the United Kingdom than the east (Fig. 6b). This is probably due to higher precipitation rates in the west leading to higher soil water contents. In the model, higher soil water content leads to two contrasting effects on N_2O emissions; firstly, the denitrification rate increases exponentially as the soil water content increases, and secondly, the proportion of denitrified N emitted as N_2O decreases linearly as soil water content increases. The exponential increase in the first process outweighs the linear decrease of the second process, leading to a simulated net increase in N_2O emissions as soil water content increases. This response reflects empirical evidence for N_2O emissions increasing as soil water content increases (e.g. Schindlbacher *et al.*, 2004; Luo *et al.*, 2013). The greater reductions in N_2O following conversion from rotational crops in the west of the country are, therefore, likely due to higher precipitation rates leading to higher soil water contents and in turn, higher N_2O emissions. Reductions in N fertilizer inputs in high precipitation grid cells will therefore lead to greater beneficial reductions in N_2O emissions.

The initial conversion of forest to pasture and crop-land (Smith & Conen, 2004) and permanent grass to bioenergy crops (Gelfand *et al.*, 2011; Nikiema *et al.*, 2012; Palmer *et al.*, 2013; Zenone *et al.*, 2015) causes a large initial N_2O emission. Our results show a large emission of N_2O in the first 5 years after conversion from permanent grass and forest to all bioenergy crops. This arises due to the simulation of cultivation during LUC from permanent grass and forest due to soil disturbance increasing soil organic matter mineralization rates. After 5 years, the modelled rates of change in N_2O emissions decline. The large initial rates of N_2O emissions arise for similar reasons to the large SOC decreases that follow certain conversions; initial cultivation of land during LUC physically fragments and redistributes soil organic matter, accelerating its decomposition, releasing inorganic N that is used by denitrifying soil microbes leading to N_2O release (Grandy & Robertson, 2006). The subsequent slowing down of increases in N_2O emissions occurs as the rapidly decomposing soil organic matter resulting from cultivation becomes depleted and the N_2O emissions move towards the background rate. Changes in N_2O

emissions following conversions from permanent grass to OSR, *Miscanthus*, SRC and SRF start to level off and decrease after approximately 5 years. This occurs because the modelled N fertilizer inputs to OSR, *Miscanthus*, SRC and SRF are lower than for permanent grass. Recent work with *Miscanthus* demonstrates that the yield benefits of N fertilization were very small and in terms of GHG emissions did not offset increased soil N_2O emissions (Roth *et al.*, 2015).

Changes in CH_4 emissions

The simulated CH_4 fluxes are very small for all land-use transitions throughout the simulation area. Owing to the absence of data for water table depth, we assumed that all soils in the simulations are freely drained, with no water table. This assumption could result in some uncertainty in the simulated CH_4 fluxes because CH_4 emissions are much higher from saturated than unsaturated soils (Segers, 1998). In the United Kingdom, observed CH_4 fluxes are much higher on organic soils (which are typically poorly drained in their natural state) than on mineral soils and are the main source of soil CH_4 emissions (Levy *et al.*, 2012). Highly organic soils (and therefore the greatest sources of CH_4) were excluded by the UKERC constraints mask from the simulations because they are unsuitable for growing bioenergy crops.

Moreover, even if significant areas of poorly drained land with high CH_4 emissions are present within the simulated area, large changes in those CH_4 emission rates resulting from conversion to bioenergy crops are only likely to occur if the land is drained for bioenergy crops. We are not aware of any planned or actual drainage of extensive areas of land for bioenergy crops. Drainage is unlikely to take place on soils currently under rotational crops because the land will already have been drained (if it was necessary). Also, SRC willow and poplar are suitable for planting on soils with a shallow water table (1–2 m deep), with willow able to cope with water-logging, making it suitable for planting in areas with a high water table or areas prone to flooding (Hall, 2003). SRC therefore provides a bioenergy option that is unlikely to require the drainage of water-logged land.

For the reasons described above, the uncertainty in the CH_4 emissions associated with the assumption of a freely draining soil is relatively small and simulated CH_4 fluxes are representative of the land suitable for bioenergy conversion. However, if extensive areas of water-logged land were to be drained for the establishment of bioenergy crops, it would be useful to explore the impacts on CH_4 fluxes (and changes in SOC and N_2O emissions) in more detail.

Effects of soil

The ECOSSE model requires input data for several soil properties: initial SOC content, pH, bulk density and clay content. These properties influence a range of processes within the model.

SOC content influences the amount of C lost as CO₂ during decomposition. All other factors being equal, soils with high organic C content will produce proportionally higher CO₂ emissions than a soil with low organic C content. We therefore expect soils with high organic C content to show greater sensitivity to changes in SOC resulting from LUC (e.g. due to cultivation). However, whilst the absolute loss of C due to cultivation is expected to be higher in soils with high organic C content, the relative loss of C may be lower if the clay content is higher.

SOC content increases as the clay content increases (Burke *et al.*, 1989). This increase occurs because clay particles strongly adhere to organic matter slowing down the decomposition process, and because clay forms aggregates that physically protect SOC from microbial decomposition (Rice, 2002). In ECOSSE, the effects of clay content on soil organic matter decomposition is modelled by altering the proportion of C released as CO₂ during decomposition (i.e. the efficiency of decomposition). As clay content increases, a smaller proportion of decomposed C is lost as CO₂ (i.e. the efficiency of decomposition increases), and a greater proportion is retained in the biomass and humus soil organic matter pools. Therefore, when clay-rich soils are cultivated during LUC (causing a large proportion of SOC to be moved from soil organic matter pools with a faster turnover rate to soil organic matter pools with a slower turnover rate), we would expect the modelled relative SOC losses to be lower than for soils with low clay content. This behaviour is in agreement with empirical evidence (e.g. Burke *et al.*, 1989).

A significant effect of soil pH on the rate of decomposition has been observed in many studies (e.g. Hall *et al.*, 1998; Andersson & Nilsson, 2001). In ECOSSE, the pH rate modifier for aerobic decomposition decreases linearly as pH drops below 4.5. For pH values >4.5, the rate modifier is set to 1 (i.e. has no effect upon the decomposition rate). Soils with a pH of <4.5 are typically highly organic. We therefore expect variations in pH between soil types to have very little impact on the model outputs because highly organic soils have been excluded from the simulation area.

In ECOSSE, bulk density affects the rate of CH₄ oxidation (i.e. consumption of CH₄). Empirical evidence shows that soils with a low bulk density tend to have higher rates of CH₄ oxidation (Borken & Brumme, 1997) because low bulk density soils are more permeable,

allowing atmospheric CH₄ and oxygen to diffuse more freely into the soil (Dörr *et al.*, 1993). Variation in bulk density in the simulated soils is very unlikely to have a significant effect on the results because (a) peat soils, which have a much lower bulk density (and therefore much higher potential oxidation rates than mineral soils), have been excluded from the simulation; (b) the simulated soil CH₄ production rates are very low so it is not possible for oxidation of CH₄ to significantly affect the net GHG balance.

Rotational grass

The permanent grass land-use type used in these simulations represents permanent, uncultivated grassland. Grassland, however, may also be temporary, used in rotation with arable crops, and in these circumstances can be regarded as a crop within an arable rotation. Permanent grassland is the most abundant type of grassland in the United Kingdom, covering 5.3 million ha in 2010, compared to 1.1 million ha of temporary (mostly rotational) grassland (Khan *et al.*, 2011) at any one time. Rotational grassland in any given year would be categorized as arable crops in different years, so the 1.1 million ha in any year represents a snapshot of the area of rotational grass. As such, rotational grass is not a land use; it is simply one component of rotational farming, which includes all-arable rotations as well as grass-arable rotations. Rotational grassland is usually represented as a crop within a rotation in most existing soil organic matter models and in ECOSSE is assumed to be a subset of arable rotational land. Permanent grassland represents a separate land-use transition as this land is only used for grass/livestock production. Rotational grass (by definition) occurs on the same land as is used for growing arable crops, so bioenergy conversion on rotational grass is equivalent to removal of land used for arable production. Rotational grassland can therefore be simulated in ECOSSE in the same way as arable-only rotations.

It is expected that rotational grassland would behave in a similar way to arable land in terms of net GHG response to LUC to bioenergy crops because a) it undergoes frequent cultivation and b) it typically receives more fertilizer than permanent grassland. This expectation is supported by empirical evidence. Long-term experiments at the Woburn Research Station (run by Rothamsted Research) in the United Kingdom found that conversion of continuous arable to rotational grassland (in this case either a 3-year grass or grass-clover ley followed by two arable crops in a 5-year cycle), resulted in only a 10–15% increase in SOC after 60 years (Johnston *et al.*, 2009). By contrast, the conversion of arable land to permanent grassland at the Rothamsted

Research Station resulted in a doubling of organic matter (indicated by total N), in 50 years (Johnston *et al.*, 2009). The small observed increase in SOC under rotational grassland suggests that the response of rotational grassland to LUC would fall between that of arable and permanent grass, but will be close to the all-arable rotations represented by our rotational crops category.

Uncertainty

There are a number of uncertainties associated with the modelled GHG balances. Uncertainty in national scale simulations has two components; uncertainty arising from the model and uncertainty arising from reduced detail and precision in data available at national scale compared to data available at the field scale. Uncertainty arising from the model was estimated as part of the site-specific modelling exercise reported in Dondini *et al.* (2015, 2016a,b). Here, we focus on uncertainties arising from the use of national scale data.

Uncertainty due to spatial and temporal resolution. The spatial and temporal resolutions of the driving data sets are given in Table 4. Due to the reduced detail of the inputs, the uncertainty in simulations at the national scale is likely to be greater than at the field scale. For example, in croplands, detailed management factors such as sowing date and timing and rate of fertilizer applications cannot usually be specified when the resolution of the simulations is larger than the size of the management unit. The resolution of the simulation here was a 1 km² grid cell, whereas the size of a management unit might be a 5 ha (0.05 km²) field, so there will be many different values for the management factors within each 1 km² cell. For example, the rate of N

Table 4 Spatial and temporal resolution of driving datasets used in the spatial simulations

Input data	Spatial resolution	Temporal resolution
Harmonised World Soil Database	30 arc s (approx. 1 km grid cells)	N/A
UKCP09 climate projections	25 km grid cells	30-year averages
Crop yield	NUTS 1 regional averages for wheat, and oilseed rape, national average for sugar beet; 1 km grid cells for <i>Miscanthus</i> , SRC and SRF, 25 km grid cells for permanent grass and forest	Annual

fertilizer application to grassland varies considerably according to the clover concentration in the grass sward, livestock stocking density and soil N status (Defra, 2010).

Uncertainty in national scale simulations is also greater than at field scale due to the reduced precision of the input data. For example, the C content of the soil in a 5 ha field can be precisely measured and the error in the measurement defined using replicates, whereas at the national scale the soil C content for grid cells is estimated from typical or averaged soil C values for the major soil types identified in the cell (e.g. Batjes, 2009).

The uncertainty due to the reduced detail and precision of data available at the national scale can be quantified by evaluating the model at field scale, but using input drivers that are available at national scale (as performed for the error bars in Fig. 7).

Uncertainty due to soil. The uncertainty associated with the use of national scale soil data was quantified by simulating 40 paired land-use transition sites (Rowe *et al.*, 2016), using measured soil parameters and soil parameters obtained from the HWSD. A statistical analysis (data not shown) of simulations using the HWSD inputs across the 40 field sites shows that there was a good correlation between modelled and measured SOC (0–100 cm depth), when using the measured soil parameters ($r = 0.92$), and when using the HWSD parameters ($r = 0.79$). In both cases, there was no significant model error and no significant model bias.

Due to the nature of the HWSD data, where the locations of soils within each grid cell are unknown, it is not possible to define which HWSD soil type corresponds to a given field site, or whether the soil type of the field site is within the dominant soils reported in the HWSD. Despite this, there was a good correlation between modelled and measured values and a lack of model bias when using HWSD parameters as inputs. This suggests that uncertainty in model results arising from the use of HWSD data is fairly small.

A similar evaluation of national scale uncertainty using ECOSSE and National Soils Inventory of Scotland soil data to simulate SOC at 60 resampled field sites in Scotland was carried out by Smith *et al.* (2010b). That study found a very strong correlation between modelled and measured SOC ($r = 0.97$). The correlation was higher in the Smith *et al.* (2010b) study than the current study ($r = 0.97$ vs. $r = 0.79$). Smith *et al.* (2010b) obtained a higher correlation probably because the soil type at each field site could be matched to the corresponding soil type in the national soil database they used.

Initial land use was estimated from the LCM2007 data at 100 m resolution which was aggregated by mode to

1 km resolution to match the HSWD data. However, as the HSWD assigns up to 10 soil types and their proportion to each 1 km × km cell, it is not spatially explicit so that matching a soil type to land use could be ambiguous as we are only considering one initial land use per grid block and not considering the proportion of each land cover in the cell. In addition, land cover is usually associated with a soil type, for example podzols with forest and brown earths with arable land, and with the data available this level of detail and precision is not possible. In this way, a small number of unlikely combinations of soil type and initial land use may have been included in the average grid results. This will need future work to resolve.

Uncertainty due to yield. Climate variability and changes in the frequency and severity of extreme events can have significant, nonlinear impacts on crop yields because crops exhibit threshold responses to stress factors (Porter & Semenov, 2005; Trnka *et al.*, 2014). Therefore, the lack of short-term climate variation in the UKCP09 climate projections presents a potentially large source of uncertainty in the predicted yields and, subsequently, the bioenergy GHG balances (Hastings *et al.*, 2009).

None of the yield models used in this study explicitly account for the effects of atmospheric N deposition on productivity; all considered the yield with optimum N supply and the crops were not, therefore, N limited. Within the simulated area of the United Kingdom, N deposition typically adds between 10 and 30 kg N ha⁻¹ yr⁻¹ (Fowler *et al.*, 2004). However, we do not expect this level of N input to significantly affect the ECOSSE model outcomes for two reasons. Firstly, the yield models have been calibrated using UK field measurements of crops subjected to atmospheric N deposition, so the effects of N deposition are to some extent implicitly captured by the models. Secondly, farmers may adjust the rates of N fertilizer applied to crops according to the N deposition rate (Jones *et al.*, 2014). For example, UK wheat farmers are advised to increase their Soil N Supply index by 20 kg N ha⁻¹ to allow for N deposition and the Defra Fertiliser Manual (Defra, 2010) factors in atmospheric N deposition (HGCA, 2009). Therefore, in fertilized cropping systems, the effects of N deposition may be largely mitigated by adaptation of fertilizer practices.

Levels of atmospheric N deposition in the United Kingdom are currently in decline due to reduced N emissions (Jones *et al.*, 2014), which could lead to reduced crop productivity. However, it is expected that fertilizer and other crop management practices will adjust to compensate for this reduction and so maintain the yields predicted by the models.

Further uncertainty arises because the crop yield projections are derived from several different sources which vary in spatial resolution, and, in the case of modelled values, the level of sophistication of the model. For example, the wheat and OSR yields are based on Defra average yield statistics for 12 regions in the United Kingdom (the NUTS level 1 regions), whereas sugar beet yields are based on a single national average yield value. Future wheat, OSR and sugar beet yields are obtained by modifying the baseline yield observations with a simple, empirical model, Miami (Lieth, 1975), whereas *Miscanthus* yield projections are obtained using a more complex, process-based model, MisanFor (Hastings *et al.*, 2009).

The crop yield projections are based on models that are parameterized and calibrated for existing cultivars and current management practices. However, crop breeding and improvements in management practices will likely lead to increases in crop yield over time (Allwright and Taylor, 2015). In addition, the yield models do not consider the impact of pests and disease, nor extreme weather events.

These sources of uncertainty in yield forecasts are difficult to quantify, either due to lack of data (e.g. changes in the frequency of extreme climate events), or because they are inherently uncertain (e.g. impacts of future crop breeding), although it is likely that an increase in crop yield of 10% per decade would not be unreasonable for these largely unimproved crops and this could have a significant impact on model outputs (Allwright and Taylor, 2016). Because these uncertainties and their impact on GHG balance estimates we tested the sensitivity of the bioenergy GHG balances to changes in yields. The main findings from this sensitivity analysis were (a) for conversions from permanent grass and forest, yield increases of up to 50% were not sufficient to change a mean detrimental change in SOC to a mean beneficial change in SOC; (b) yield increases of up to 50% of any given bioenergy crop were generally insufficient to alter the crop's ranking in terms of changes in SOC, even when the yields of all other bioenergy crops were left unchanged; and (c) SRF and *Miscanthus* showed the greatest sensitivity to proportional changes in yield because they have the highest yields within the simulated area.

Although changes in estimated yields would certainly affect the total area of land favourable for conversion to bioenergy crops, our findings suggest that the broad conclusions inferred from the modelling results would remain unchanged.

Uncertainty due to fertilizer use. A large number of factors affect the amount of N fertilizer applied to a crop including the soil N status, expected crop N demand,

weather, soil texture, regulations (e.g. in nitrogen vulnerable zones) and economic factors (e.g. cost of fertilizer). For grassland, additional factors may include the percentage of clover in the grass sward and stocking density. Many of these factors vary at a finer scale than the 1 km resolution of the simulations and are not described in any spatially defined databases. Therefore, the model makes assumptions about the amount of N fertilizer applied, which presents a source of uncertainty for the modelled changes in N₂O emissions.

To quantify this uncertainty, we conducted a sensitivity analysis to explore the impacts of a ±20% variation to the default N fertilizer application rate in a sample of the grid cells. The results of this analysis (data not shown) show that transitions to wheat were most sensitive to a proportional change in N fertilizer inputs: a 20% increase in N fertilizer led to a mean increase in N₂O emissions of about 5 t CO₂e ha⁻¹ after 35 years (i.e. in 2050) and a 20% decrease reduced N₂O emissions by about 5.5 t CO₂e ha⁻¹. Other transitions showed mean deviations in N₂O emissions within ±2.5 t CO₂e ha⁻¹. The shifts in N₂O emissions resulting from a ±20% change in N fertilizer rates are modest, leading to a <5% change in the mean net GHG balance of each transition. Therefore, we do not expect uncertainty around N fertilization rates to be a source of large uncertainty in the modelling outcomes.

Future research needs

This study shows that future work should target second-generation bioenergy crops (*Miscanthus*, SRC and SRF), because these offer a much more favourable net GHG balance than first-generation bioenergy crops (wheat, sugar beet and OSR). It is noteworthy, however, that the overall GHG balance of bioenergy may still be positive, even if there are net preharvest soil GHG emissions due to land-use change, and the full value chain needs to be considered (Newton-Cross & Evans, 2015).

Whilst the type of land-use transition was the most important factor affecting net GHG balance, crop yield was found to be the most influential factor within each type of transition. However, a number of limitations of the yield data constrain the spatial accuracy of the soil GHG balance predictions and should be the focus of future research.

Firstly, Defra yield data for wheat (also used for the baseline rotational crop yield), sugar beet and OSR are spatially coarse, being available only at regional level, and only cover a short time span. The development of high-resolution spatial datasets of bioenergy crop yield would greatly improve the spatial accuracy of net GHG balance predictions.

Development of yield models is often hampered by lack of detailed soil and plant data from which to formulate process descriptions and evaluate the model. For example, only 11 UK experimental sites with sufficient data to validate the MiscanFor model were available (Hastings *et al.*, 2009). Future research should place an emphasis on detailed, long-term measurements of crop and soil attributes (yield, litter inputs, C and N contents of plant components and soil etc.), over the full life cycle of the crop, for the latest germplasm released from breeding programmes. Such data are required for the development of more robust and improved parameterizations of process-based models, critical for future predictions.

Models of future crop yield vary in the factors they take into account. For example (e.g. effects of elevated atmospheric CO₂ concentration), their level of sophistication and degree to which they have been calibrated for UK conditions. Moreover, where multiple models exist for a given crop, the yield estimates may differ considerably. For example, MiscanFor (Hastings *et al.*, 2009) predicts the highest *Miscanthus* yields to be in the south-west of England, whereas the empirical model of Richter *et al.* (2008) predicts relatively low yields in the south-west. Further work on model evaluation and model comparison is required to resolve these differences and reduce the uncertainty in model estimates. In the short-term, the uncertainty associated with choice of model could be quantified by modelling net GHG balance using yield forecasts produced from an ensemble of yield models for each crop.

Overall, the reliability and spatial accuracy of future net GHG balance modelling would benefit greatly from improvements in bioenergy yield modelling (or direct modelling of crop inputs of C to the soil). Standardization of yield models for different crops, such as the effect of soil type on soil water capacity, would enable more reliable comparison of different land-use transitions.

Finally, little is known about the impact of bioenergy crop re-establishment on SOC. Different re-establishment techniques involve different amounts of soil disturbance, which could lead to enhanced soil organic matter decomposition rates. Soil disturbance from re-establishment could have a significant effect on long-term C sequestration, with a proportion of the C sequestered during the previous planting cycle being lost again as CO₂ to the atmosphere (Grogan & Matthews, 2002). Research into the practicality of a range of potential re-establishment techniques and their impacts on soil C dynamics should be a high priority.

In conclusion, we have shown that increasing yield increases SOC so that in addition to optimizing the use of land, and obtaining the highest energy yield per unit

area, research into improving the yield of SRC, SRF and *Miscanthus* genotypes will provide benefits to both energy security and GHG mitigation. When assessing the full GHG impacts of energy crops, all components of the bioenergy value chain (e.g. cultivation, management, harvest, transportation, processing, fossil fuel offset GHG impacts) need to be considered (Newton-Cross & Evans, 2015). The findings presented here fill the critical gap in preharvest GHG emission data, used to assess the full life cycle GHG emissions from energy crops in bioenergy value chains.

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